# SLAKCH REQUEST FORM

Scientific and Technical Information Center Mail Box and Bldg/Room Location: 2 Results Format Preferred (circle): PAPER DISK E-MAIL If more than one s arch is submitted, please prioritize search s in order of need. Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract. Title of Invention: Inventors (please provide full names): Earliest Priority Filing Date: \*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number. Please search structures of attached dain 33 in all patent & mon-patent databases Technical Info. Specialist CM1 12D16 Tel: 308-4258 Note - nwiety denoted Please provide all hits, it possible. act garagella Type of Search Vendors and cost where applicable Searcher Location: Questel/Orbit Date Searcher Picked Up: Bibliographic Litigation Searcher Prep & Review Time: Fulltext Clerical Prep Time: Patent Family Online Time: 1101 PTO-1590 (1-2000)

BEST AVAILABLE COPY

Lacca 884813

-11.76

ENTRY -11.76

CA SUBSCRIBER PRICE

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STRUCTURE FILE UPDATES: 4 APR 2001 HIGHEST RN 330150-69-1 DICTIONARY FILE UPDATES: 4 APR 2001 HIGHEST RN 330150-69-1

TSCA INFORMATION NOW CURRENT THROUGH July 8, 2000

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

=> d 116 que stat; s 116 or 116; d 9000 18000 reg

T: VAR G1=32-2 33-29/34-2 35-29/38-2 40-29/N/O/S/SE/44-2 45-29
T: VAR G2=32-4 33-30/34-4 35-30/38-4 40-30/N/O/S/SE/44-4 45-30
T: VAR G3=32-6 33-31/34-6 35-31/38-6 40-31/44-6 45-31/N/O/S/SE
NODE ATTRIBUTES:

NSPEC IS RC AT 29
NSPEC IS RC AT 30
NSPEC IS RC AT 31
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 26
Prepared by M. Hale 308-4258

Page 234

STEREO ATTRIBUTES: NONE

18388 SEA FILE=REGISTRY SSS FUL L14 L16

100.0% PROCESSED 65653 ITERATIONS

SEARCH TIME: 00.00.12

18388 ANSWERS

L23 18388 L16 OR L16

9000 RN 147113-41-5 REGISTRY 18000 RN 39069-69-7 REGISTRY

=> s 123 range=(147113-41-5,)

L24 9000 L16 OR L16

\s 12∂\rang**e**\(38069-69-

=> del 125 y;s 123 range=(39069-69-7,147113-41-5)

L25 9001 L16 OR L16

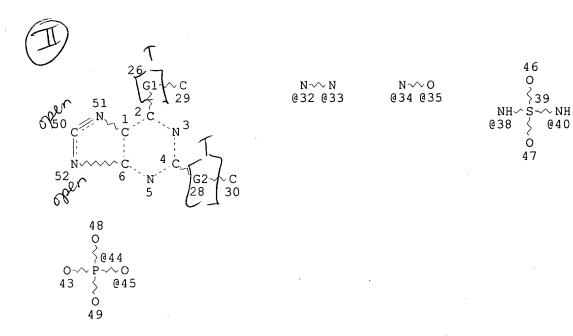
=> s 123 range=(,39069-69-7)

389 L16 OR L16 L26

=> d 119 que stat;d 122 que stat;fil medl,caplus,biosis,embase;s (124 or 125)

and 119 and 122

L17 STR



T-, VAR G1=32-2 33-29/34-2 35-29/38-2 40-29/N/O/S/SE/44-2 45-29 VAR G2=32-4 33-30/34-4 35-30/38-4 40-30/N/O/S/SE/44-4 45-30 NODE ATTRIBUTES:

NSPEC IS RC

ΑT 29

IS RC AT 30

DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE

4933 SEA FILE=REGISTRY SSS FUL L17

100.0% PROCESSED 10151 ITERATIONS

SEARCH TIME: 00.00.12

4933 ANSWERS

L20

STR



VAR G2=32-4 33-30/34-4 35-30/38-4 40-30/N/O/S/SE/44-4 45-30 NODE ATTRIBUTES: AT 30 NSPEC IS RC DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

49

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

307 SEA FILE=REGISTRY SSS FUL L20

100.0% PROCESSED 13563 ITERATIONS 307 ANSWERS

SEARCH TIME: 00.00.11

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 406.89 1649.65 FULL ESTIMATED COST DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -11.76

FILE 'MEDLINE' ENTERED AT 13:53:05 ON 06 APR 2001

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Page 237

@40

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<---->u u SEARCH ENDED BY USER

=> s (124 or 125) and 119 and 122

L27 0 FILE MEDLINE
L28 1 FILE CAPLUS
L29 0 FILE BIOSIS
L30 0 FILE EMBASE

TOTAL FOR ALL FILES

L31 1 (L24 OR L25) AND L19 AND L22

=> d cbib abs hitstr

# L31 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2001 ACS

2000:241135 Document No. 132:279106 Non-peptide GnRH agents, methods and intermediates for their preparation. Anderson, Mark Brian; Vazir, Haresh N.; Luthin, David Robert; Paderes, Genevieve Deguzman; Pathak, Ved P.; Christie, Lance Christopher; Hong, Yufeng; Tompkins, Eileen Valenzuela; Li, Haitao; Faust, James (Agouron Pharmaceuticals, Inc., USA; et al.). PCT Int. Appl. WO 2000020358 A2 20000413, 444 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-US18790 19990820. PRIORITY: US 1998-97520 19980820.

GΙ

$$R^{5}$$
  $R^{1}$   $R^{2}$ 

Het-X  $R^{8}$ 
 $R^{7}$   $R^{8}$ 
 $R^{4}$   $R^{9}$ 

AB Non-peptide GnRH agents capable of inhibiting the effect of gonadotropin-releasing hormone are described. The compds. and their pharmaceutically acceptable salts, multimers, prodrugs, and active metabolites are suitable for treating mammalian reproductive disorders

and

steroid hormone-dependent tumors as well as for regulating fertility, where suppression of gonadotropin release is indicated. The compds. include those of formula I [X = C:O, C:S, S:O, or SO2; Het = 5-membered NOS-heterocycle; R1, R2 = H, alkyl; R3-R7 = H, halo, (un)substituted alkyl, aryl, heteroaryl, CH2OR, OR, CO2R; R = alkyl, aryl, etc.; adjacent rings positions such as R6R7 may form (un)substituted 5- or 6-membered ring with up to 4 heteroatoms; R8 = lipophilic moiety such as alkyl,

II

aryl,

CH2OR, OR, etc.; R9 = H, (un)substituted alkyl]. Methods and intermediates for synthesizing the compds. are also described. For instance, 4,4,7-trimethylchroman (prepn. given) was alkylated in the 6-and 8-positions using Et 5-(chloromethyl)-2-furoate (46% total yield),

and

the resulting esters were hydrolyzed to a mixt. of acids. This unsepd. mixt. was treated with  ${\tt SOCl2}$  and amidated with

2,4,6-trimethoxyphenylamine-

HCl to give the invention compd. II and its chroman-6-position isomer, which were sepd. by HPLC. Several compds. exhibited high affinity (<100 nM) at human GnRH receptors. The compds. antagonized GnRH-stimulated inositol phosphate accumulation in cells with recombinant human GnRH receptors, and an example compd. reduced plasma LH levels in castrated male rats. Various biol. data for several hundred compds. are given.

IT 263848-23-3P 263851-39-4P 263857-23-4P 263857-27-8P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of non-peptide GnRH agents for regulating Prepared by M. Hale 308-4258 Page 239

gonadotropin secretion)

RN 263848-23-3 CAPLUS

CN 2-Furancarboxamide,

N-[[4-[[(4,6-dimethoxy-2-pyrimidinyl)amino]methyl]cycl ohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

RN 263851-39-4 CAPLUS

CN 2-Furancarboxamide, N-[2-(dimethylamino)-1H-purin-6-yl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

RN 263857-23-4 CAPLUS

CN 2-Furancarboxamide, N-(6,7-dihydro-6-oxo-1H-purin-2-yl)-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

Me Me 
$$CH_2$$
  $O$   $C$   $NH$   $N$   $NH$ 

RN 263857-27-8 CAPLUS
CN 2-Furancarboxamide,
N-(4,6-dimethoxy-2-pyrimidinyl)-5-[(5,6,7,8-tetrahydro3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

### => fil reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	1401.60	3051.25
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	$\mathtt{TOTAL}$
•	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.59	-12.35

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Structure search limits have been increased. See  $\ensuremath{\mathsf{HELP}}$  SLIMIT for details.

=> e malonato/cn 5

Prepared by M. Hale 308-4258

```
MALONATE-TRANSPORTING PROTEIN (PSEUDOMONAS PUTIDA GENE
E1
              1
MDCL)
                     /CN
                    MALONATE-TRANSPORTING PROTEIN (PSEUDOMONAS PUTIDA GENE
E2
              1
MDCM)
                     /CN
              0 --> MALONATO/CN
E3
                    MALONATO 1,2-DIAMINOCYCLOHEXANE PLATINUM(II)/CN
E4
              1
                    MALONATO O-PHENYLENEDIAMINE PLATINUM(II)/CN
E5
=> dis his
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     FILE 'REGISTRY' ENTERED AT 13:31:06 ON 06 APR 2001
L1
                 STR
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L2
                      /FUL
           17170 S L1
L3
           17170 S L3
                      OR L3
L4
            9000 S LA
                       RAN=(135867-73
<u>L</u>5
            8171 S 14
                       RAN = (, 135/867 - 7/3 - 1)
L6
                                      EMBASE'
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17
1/8
              20 FILE CAPLUS
L/9
               O FILE BIOSIS
T#0
               O FILE EMBASE
     TOTAL FOR ALL FILES
              20'S (L5 OR L6) (L) (MIXT OR MIX?)
     FILE 'REGISTRY' ENTERED AT 13:39:50 ON 06 APR 2001
                 STR L1
L12
              50 S L12
L13
L14
                 STR L12\
              50 S L14
L15
L16
          18388 S L14 FUL
L17
                 STR L14
              50 S L17
L18
            4933 S L17 FUL
L19
L20
                 STR L17
              19 S L20
L21
L22
             307 S L20 FUL
          18388 S L16 OR L16
L23
                         RAN = (147113 - 41 - 5,)
            9000 S L23
L24
                         RAN=(39069-69-7,147113-41-5)
            9001 S L23
L25
             389 S L23
                         RAN=(,39069-69-7)
L26
     FILE 'MEDLINE, CAPLUS, BIOSIS, EMBASE' ENTERED AT 13:53:05 ON 06 APR 2001
L27
               O FILE MEDLINE
               1 FILE CAPLUS
L28
               O FILE BIOSIS
L29
L30
               O FILE EMBASE
     TOTAL FOR ALL FILES
               1 S (L24 OR L25) AND L19 AND L22 Prepared by M. Hale 308-4258
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Page 242

L31

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FILE 'REGISTRY' ENTERED AT 13:57:06 ON 06 APR 2001
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               1 S E4
L32
                 STR
L33
L34
              50 S L33
                 E MALONATE/CN 5
L35
               1 S E3
                 E PYRROLIDINYL/CN 5
                 E PYRROLIDINE/CN 5
L36
               1 S E3
                 E PIPERIDINE/CN 5
               1 S E3
L37
                 E PIPERIDINYLMETHYLENE/CN 5
                 E MORPHOLINE/CN 5
               1 S E3
L38
L39
                 STR L14
L40
              36 S L39
                 BATCH SSS FUL L40 GARCIAPT1/B
L41
                 STR L17
L42
              35 S L41
L43
            5070 S L41 FUL
                 SAVE L43 GARCIAPT2/A
L44
                 STR L20
L45
               6 S L44
L46
             314 S L44 FUL
                 SAVE GARCIAPT3/A L46
=> d 143 que stat;d 146 que stat;fil medl,caplus,biosis,embase;s 143 and 146
                 STR
L41
                                 46
                                                  48
                                                  0
                                 0
  N \sim N
                N\sim\sim O
                                                  S@44
                                 39
               034 035
 @32 @33
                             NH~S~NH
                                              0 \sim P \sim 0
                            038
                                    @40
                                              43
                                                     045
                                 0
                                                  0
                                 47
                                                  49
                                             59
                                     58
          26
                                     0
                                             0
                                 0~~ C~
                                        ∨CH2-C-\O
                                053 54 55 56 057
                   G2√ C
                   28
                       30
```

VAR G1=32-2 33-29/34-2 35-29/38-2 40-29/N/O/S/SE/44-2 45-29/HY/53-2 57-29 VAR G2=32-4 33-30/34-4 35-30/38-4 40-30/N/O/S/SE/44-4 45-30/HY/53-4 57-30 NODE ATTRIBUTES:

NSPEC IS RC AT 2

Prepared by M. Hale 308-4258

Page 243

NSPEC IS RC AT 30 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 34

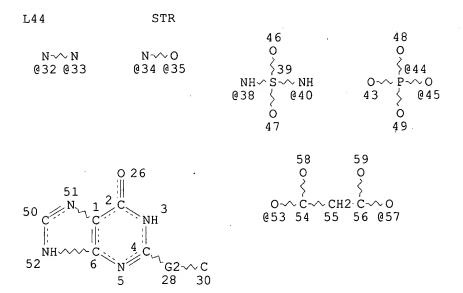
STEREO ATTRIBUTES: NONE

L43 5070 SEA FILE=REGISTRY SSS FUL L41

100.0% PROCESSED 139298 ITERATIONS

5070 ANSWERS

SEARCH TIME: 00.00.25



VAR G2=32-4 33-30/34-4 35-30/38-4 40-30/N/O/S/SE/44-4 45-30/HY/53-4 57-30 NODE ATTRIBUTES:
NSPEC IS RC AT 30

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 33

STEREO ATTRIBUTES: NONE .

L46 314 SEA FILE=REGISTRY SSS FUL L44

100.0% PROCESSED 78598 ITERATIONS

SEARCH TIME: 00.00.16

314 ANSWERS

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

299.51 3350.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE

0.00 -12.35

FILE 'MEDLINE' ENTERED AT 14:09:35 ON 06 APR 2001

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L47 0 FILE MEDLINE
L48 46 FILE CAPLUS
L49 0 FILE BIOSIS
L50 0 FILE EMBASE

TOTAL FOR ALL FILES

L51 46 L43 AND L46

=> s 151(l) (mixt? or cook p?/au or combinator?)

TOTAL FOR ALL FILES

L56 6 L51(L) (MIXT? OR COOK P?/AU OR COMBINATOR?)

=> d 1-6 cbib abs hitstr

L56 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2001 ACS
2000:384565 Document No. 133:28236 Methods and compositions for performing
an array of chemical reactions on a support surface. Zebala, John A.
(Syntrix Biochip, Inc., USA). PCT Int. Appl. WO 2000033084 A2 20000608,
Prepared by M. Hale 308-4258

157 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-US28021 19991123. PRIORITY: US 1998-PV110527 19981201; US 1999-326479 19990604. Compns. and methods are provided for performing regionally selective

AB Compns. and methods are provided for performing regionally selective solid-phase chem. synthesis of org. compds. Such methods may employ solvent-resistant photoresist compns. to prep. arrays of org. compds., such as ligands, for use within a variety of diagnostic and drug discovery

assays. Ligand-arrays may comprise, for example, nucleobase polymers that

are resistant to degradative enzymes. DNA probes and enalaprilat analogs were synthesized on glass slides using a photoresist method and used in hybridization assays and ACE inhibitory activity screening.

IT 1445-15-4 10030-78-1 20758-33-2

RL: DEV (Device component use); PRP (Properties); USES (Uses) (array of nucleobase polymers contg.; methods and compns. for performing arrays of chem. reactions on support surfaces using photoresists)

RN 1445-15-4 CAPLUS

CN 6H-Purin-6-one, 2-(dimethylamino)-1,7-dihydro- (9CI) (CA INDEX NAME)

RN 10030-78-1 CAPLUS

CN 6H-Purin-6-one, 1,7-dihydro-2-(methylamino)- (9CI) (CA INDEX NAME)

RN 20758-33-2 CAPLUS

CN 1H-Purin-6-amine, N-(3-methyl-2-butenyl)-2-(methylthio)- (9CI) (CA INDEX NAME)

GI

L56 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2001 ACS 2000:241135 Document No. 132:279106 Non-peptide GnRH agents, methods and intermediates for their preparation. Anderson, Mark Brian; Vazir, Haresh N.; Luthin, David Robert; Paderes, Genevieve Deguzman; Pathak, Ved P.; Christie, Lance Christopher; Hong, Yufeng; Tompkins, Eileen Valenzuela; Li, Haitao; Faust, James (Agouron Pharmaceuticals, Inc., USA; et al.). PCT Int. Appl. WO 2000020358 A2 20000413, 444 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-US18790 19990820. PRIORITY: US 1998-97520 19980820.

AB Non-peptide GnRH agents capable of inhibiting the effect of gonadotropin-releasing hormone are described. The compds. and their pharmaceutically acceptable salts, multimers, prodrugs, and active metabolites are suitable for treating mammalian reproductive disorders and Prepared by M. Hale 308-4258 Page 247

Ι

steroid hormone-dependent tumors as well as for regulating fertility, where suppression of gonadotropin release is indicated. The compds. include those of formula I [X = C:O, C:S, S:O, or SO2; Het = 5-membered NOS-heterocycle; R1, R2 = H, alkyl; R3-R7 = H, halo, (un)substituted alkyl, aryl, heteroaryl, CH2OR, OR, CO2R; R = alkyl, aryl, etc.; adjacent rings positions such as R6R7 may form (un)substituted 5- or 6-membered ring with up to 4 heteroatoms; R8 = lipophilic moiety such as alkyl,

aryl,

CH2OR, OR, etc.; R9 = H, (un)substituted alkyl]. Methods and intermediates for synthesizing the compds. are also described. For instance, 4,4,7-trimethylchroman (prepn. given) was alkylated in the 6-and 8-positions using Et 5-(chloromethyl)-2-furoate (46% total yield),

and

the resulting esters were hydrolyzed to a mixt. of acids. This unsepd. mixt. was treated with SOC12 and amidated with 2,4,6-trimethoxyphenylamine-HCl to give the invention compd. II and its chroman-6-position isomer, which were sepd. by HPLC. Several compds. exhibited high affinity (<100 nM) at human GnRH receptors. The compds. antagonized GnRH-stimulated inositol phosphate accumulation in cells with recombinant human GnRH receptors, and an example compd. reduced plasma LH levels in castrated male rats. Various biol. data for several hundred compds. are given.

IT 263851-39-4P 263857-23-4P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of non-peptide GnRH agents for regulating gonadotropin secretion)

RN 263851-39-4 CAPLUS

CN 2-Furancarboxamide, N-[2-(dimethylamino)-1H-purin-6-yl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

RN 263857-23-4 CAPLUS

CN 2-Furancarboxamide, N-(6,7-dihydro-6-oxo-1H-purin-2-yl)-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

Prepared by M. Hale 308-4258

Page 248

L56 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2001 ACS

1996:744343 Document No. 126:89695 Nucleic Acid Related Compounds. 93. A Solution for the Historic Problem of Regioselective Sugar-Base Coupling

To Produce 9-Glycosylguanines or 7-Glycosylguanines. Robins, Morris J.;

Zou,
Ruiming; Guo, Zhiqiang; Wnuk, Stanislaw F. (Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, 84602-5700, USA). J Org. Chem., 61(26), 9207-9212 (English) 1996. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT 126:89695. Publisher: American Chemical Society.

GI

AB Per(trimethylsilyl)-2-N-acylguanine derivs. and tetra-O-acylpentofuranoses

Ι

were coupled [tin(IV) chloride or titanium(IV) chloride catalysis] to give

predominant formation of 7-glycosylguanines. With TiCl4, a org./aq. partitioning allowed isolation of 7-glycosylguanines from the 7/9 isomer mixts. Per(trimethylsilyl)-2-N-acyl-6-O- (diphenylcarbamoyl)guanine derivs. and tetra-O-acylpentofuranoses underwent regioselective coupling (trimethylsilyl

trifluoromethanesulfonate catalysis) to give 9-glycosylguanines. The 6-O-(diphenylcarbamoyl)peracyl-9-.beta.-D-ribofuranosyl isomer was shown to be both the kinetic and thermodn. coupling product. Deprotection of all of the peracyl coupling products was effected under mild conditions

to

give good to high yields of guanine nucleoside analogs. These methodologies provide solns. for the regionelective prepn. of 7- and 9-glycosylguanine nucleosides, e.g. I.

IT 19962-37-9 21047-89-2

RL: RCT (Reactant)

(regioselective sugar-base coupling with nucleobases in prepn. of glycosylguanine nucleosides)

RN 19962-37-9 CAPLUS

CN Acetamide, N-(6,7-dihydro-6-oxo-1H-purin-2-yl)- (9CI) (CA INDEX NAME)

RN 21047-89-2 CAPLUS

CN Propanamide, N-(6,7-dihydro-6-oxo-1H-purin-2-yl)-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & H & H \\ I-Pr-C-NH & H & N \\ N & N & N \\ O & O \end{array}$$

IT 112233-74-6P 112233-75-7P 112233-76-8P

112233-77-9P 112233-78-0P 185610-53-1P

185610-60-0P 185610-62-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (regioselective sugar-base coupling with nucleobases in prepn. of glycosylguanine nucleosides)

RN 112233-74-6 CAPLUS

CN Carbamic acid, diphenyl-, 2-(acetylamino)-1H-purin-6-yl ester (9CI) (CA INDEX NAME)

RN 112233-75-7 CAPLUS
CN Guanosine, N-acetyl-, 2',3',5'-triacetate 6-(diphenylcarbamate) (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

RN 112233-77-9 CAPLUS CN Carbamic acid, diphenyl-, 2-(acetylamino)-9-(2,3,5-tri-O-acetyl-.beta.-D-xylofuranosyl)-9H-purin-6-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 112233-78-0 CAPLUS
CN Carbamic acid, diphenyl-,
2-(acetylamino)-9-[[2-(acetyloxy)ethoxy]methyl]9H-purin-6-yl ester (9CI) (CA INDEX NAME)

RN 185610-53-1 CAPLUS
CN Carbamic acid, diphenyl-, 2-[(2-methyl-1-oxopropyl)amino]-1H-purin-6-yl ester (9CI) (CA INDEX NAME)

RN 185610-60-0 CAPLUS
CN Guanosine, N-(2-methyl-1-oxopropyl)-, 2',3',5'-triacetate 6-(diphenylcarbamate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 185610-62-2 CAPLUS

CN Guanosine, N-acetyl-N-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-, 2',3',5'-triacetate 6-(diphenylcarbamate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## IT 185610-54-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (regioselective sugar-base coupling with nucleobases in prepn. of glycosylguanine nucleosides)

RN 185610-54-2 CAPLUS

CN Carbamic acid, diphenyl-, 2-[acetyl[[2-(acetyloxy)ethoxy]methyl]amino]-9[[2-(acetyloxy)ethoxy]methyl]-9H-purin-6-yl ester (9CI) (CA INDEX NAME)

AcO-CH2-CH2-O-CH2

L56 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2001 ACS 1995:994426 Document No. 124:87803 Preparation of substituted N-ethylglycine

derivatives for the preparation of peptide nucleic acids and peptide nucleic acid/deoxyribonucleic acid hybrids.. Breipohl, Gerhard; Uhlmann, Eugen; Knolle, Jochen (Hoechst A.-G., Germany). Eur. Pat. Appl. EP

A1 19950920, 31 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE. (German). CODEN: EPXXDW.

APPLICATION: EP 1995-103333 19950308. PRIORITY: DE 1994-4408534

PGXCH2CH2N(COYB)CH2CO2H [PG = urethane- or trityl-type protecting group labile to weak acid; X = NH, O, S; Y = CH2, NH, O; B = (protected) nucleoside (replacement) base], were prepd. Thus, N-[(4-methoxyphenyl)diphenylmethyl]aminoethylglycine Me ester (prepn. given) in DMF was treated sequentially with 3,4-dihydro-4-oxo-1,2,3-benzotriazine, 4-ethylmorpholine, N4-benzoyl-N1-carboxymethylcytosine in DMF, and with DCC; the mixt. was stirred 20 h at room temp. to give the coupling product, which was sapond. with aq. NaOH/dioxane to give N-[(4-methoxyphenyl)diphenylmethyl]aminoethyl-N-[[1-(N4-benzoyl)cytosyl]acetyl]glycine.

IT 112233-74-6

RL: RCT (Reactant)

 $% \left( \mathcal{L}_{0}\right) =\left( \mathcal{L}_{0}\right)$  (prepn. of substituted N-ethylglycine derivs. for the prepn. of peptide

nucleic acids and peptide nucleic acid/DNA hybrids)

RN 112233-74-6 CAPLUS

CN Carbamic acid, diphenyl-, 2-(acetylamino)-1H-purin-6-yl ester (9CI) (CA INDEX NAME)

IT 21047-89-2P 172405-24-2P 172405-25-3P Prepared by M. Hale 308-4258

#### 172405-26-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of substituted N-ethylglycine derivs. for the prepn. of

peptide

nucleic acids and peptide nucleic acid/DNA hybrids)

RN 21047-89-2 CAPLUS

CN Propanamide, N-(6,7-dihydro-6-oxo-1H-purin-2-yl)-2-methyl- (9CI) (CA INDEX NAME)

RN 172405-24-2 CAPLUS
CN 9H-Purine-9-acetic acid,
2-(acetylamino)-6-[[(diphenylamino)carbonyl]oxy] , methyl ester (9CI) (CA INDEX NAME)

RN 172405-26-4 CAPLUS

CN Glycine, N-[[2-(acetylamino)-6-[[(diphenylamino)carbonyl]oxy]-9H-purin-9-Prepared by M. Hale 308-4258 Page 255 yl]acetyl]-N-[2-[[(4-methoxyphenyl)diphenylmethyl]amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

IT 172405-34-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of substituted N-ethylglycine derivs. for the prepn. of peptide

nucleic acids and peptide nucleic acid/DNA hybrids)

RN 172405-34-4 CAPLUS

CN Glycine, N-[[2-(acetylamino)-6-[[(diphenylamino)carbonyl]oxy]-9H-purin-9-yl]acetyl]-N-[2-[[(4-methoxyphenyl)diphenylmethyl]amino]ethyl]- (9CI)

(CA

INDEX NAME)

L56 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2001 ACS

1975:497209 Document No. 83:97209 New synthesis of disubstituted
8-aminopurine derivatives. Yoneda, Fumio; Higuchi, Masatsugu; Hayakawa,
Akio (Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan). Synthesis (4),
264-5 (English) 1975. CODEN: SYNTBF.

GI For diagram(s), see printed CA Issue.

Aminopurines I (X = H2, R = Me, Ph, MeS, EtS) were prepd. in 80-95% yield by treating nitrosopyrimidines II with excess Me2NCH(OEt)2 (III) and then dilg. the reaction mixt. with H2O. When the reaction mixt was dild. with ether (methyleneamino)purines I (X = Me2NCH; R = Me, Ph, MeS, EtS) were obtained in 69-84% yield. Similarly treating nitrosopyrimidines IV (R = MeS, EtS) with excess III gave 40% and 45% oxopurines V (R = MeS, EtS), resp.

IT 43005-36-3P 56472-00-5P 56472-01-6P 56472-02-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

Prepared by M. Hale 308-4258

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RN 43005-36-3 CAPLUS

CN 6H-Purin-6-one, 8-(dimethylamino)-1,7-dihydro-2-(methylthio)- (9CI) (CA INDEX NAME)

RN 56472-00-5 CAPLUS

CN Methanimidamide, N'-[8-(dimethylamino)-2-(methylthio)-1H-purin-6-yl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

RN 56472-01-6 CAPLUS

CN Methanimidamide, N'-[8-(dimethylamino)-2-(ethylthio)-1H-purin-6-yl]-N, N-dimethyl- (9CI) (CA INDEX NAME)

RN 56472-02-7 CAPLUS

CN 6H-Purin-6-one, 8-(dimethylamino)-2-(ethylthio)-1,7-dihydro- (9CI) (CA INDEX NAME)

L56 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2001 ACS Prepared by M. Hale 308-4258 1970:90522 Document No. 72:90522 Polythiocyanatopurines. Saneyoshi, Mineo (Seikagaku Kogyo Co., Ltd.). Japan. JP 45002179 B4 19700124 Showa, 2 pp. (Japanese). CODEN: JAXXAD. APPLICATION: JP 19650921.

AB Reaction of a di- or trimercapto-substituted-purine with a cyanogen halide

is described. In an example, 2.12 g BrCN in EtOH is dropped into a cold (0.degree.)mixt. of 1.88 g 2,6-dimercapto-9-methylpurine and 100 ml 0.2N NaOH, the mixt. stirred at 0-5.degree. 1 hr, stirred 1 hr more with 2 ml N HCl, filtered, and the mass washed with cold H2O and EtOH to give 1.96 g 2,6-dithiocyanato-9-methylpurine, m. 240.degree. (aq. EtOH). Similarly prepd. are the following compds.: 2,8-dithiocyanato-6-hydroxypurine, m. 240.degree., 2,6,8-trithiocyanato-purine, m. 240.degree., and 6,8-dithiocyanatopurine, m. 240.degree..

IT 6220-39-9P 26821-00-1P 26821-02-3P

RN 6220-39-9 CAPLUS

CN Thiocyanic acid, 6-hydroxypurine-2,8-diyl ester (7CI, 8CI) (CA INDEX NAME)

RN 26821-00-1 CAPLUS

CN Thiocyanic acid, 9-methyl-9H-purine-2,6-diyl ester (8CI) (CA INDEX NAME)

RN 26821-02-3 CAPLUS

CN Thiocyanic acid, purine-2,6,8-triyl ester (8CI) (CA INDEX NAME)

#### => fil casrea

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	355.16	3705.92
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-3.53	-15.88

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FILE CONTENT:1985 - 1 Apr 2001 (VOL 102 ISS 1 - VOL 134 ISS 14)

- >>> Several important enhancements to CASREACT functional group <<<
- >>> searching were introduced. Enter HELP FGA or HELP FGC for more <<<
- >>> information. <<<

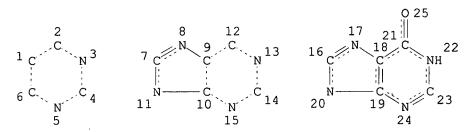
This file contains CAS Registry Numbers for easy and accurate substance identification.

Structure search limits have been increased. See HELP SLIMIT for details.

=> d 158 que stat;s 158(1) (mixt? or combinator?)

L1

STR



NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L58 326 SEA FILE=CASREACT SSS FUL L1 ( 3520 REACTIONS) Prepared by M. Hale 308-4258

Page 259

326 DOCS

SEARCH TIME: 00.00.04

21697 MIXT? 415 COMBINATOR?

L59 1 L58(L) (MIXT? OR COMBINATOR?)

=> d fhit cbibabs

'CBIBABS' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

```
The following are valid formats:
ABS ----- &I and AB
ALL ----/BIB, AB, IND, RE, Single-step Reactions
           🗲 AI, PRAI
BIB -----/- AN, plus Bibliographic Data
CAN -----/-- List of CA abstract numbers without answer numbers

←--- AN, plus Compressed Bibliographic Data

DALL --/--- ALL, delimited (end of each field identified)
IABS ----- ABS, indented with text labels IALL ----- ALL, indented with text labels IBIB ----- BIB, indented with text labels IND ----- Indexing data
IPC ----- Internationa / Patent Classifications
ISTD ---- STD, indented with text labels
OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ---- OBIB, indented with text labels
SBIB ----- BIB, no/citations
SIBIB ----- IBIB, no citations
MAX ----- Same as ALL
PATS ----- PI, SØ
SCAN ----- TI and FCRD (random display, no answer number. SCAN
             must/ be entered on the same line as DISPLAY, e.g.,
              D SCAN.)
SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for
              all single-step reactions)
STD ----- BIB, IPC, and NCL
CRD ----- Compact Display of All Hit Reactions
CRDREF ---- Compact Reaction Display and SO, PY for Reference
FHIT ----- Reaction Map, Diagram, and Summary for first
             hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ----- First hit in Compaarphit Reaction Display (CRD) format
FCRDREF ---- First hit in Compa¢t Reaction Display (CRD) format with
             CA reference information (SO, PY). (Default)
FPATH ----- PATH, plus Reacti∮n Summary for the "long path"
FSPATH ---- SPATH, plus Reaction Summary for the "short path"
HIT ----- Reaction Map, Reaction Diagram, and Reaction Prepared by M. Hale 308-4258
```

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Summary for all hit reactions and fields containing hit terms All/hit fields and the number of occurrences of the hit terms in each field. Includes total number of H/TT, PATH, SPATH reactions. Labels reactions that have fincomplete verifications. -/ Reaction Map and Reaction Diagram for the "long path". Displays all hit reactions, except those whose steps are totally included within another hit reaction which is displayed --- Hit Reactions (Map, Diagram, Summary for all hit reactions) --- Hit Reaction Graphics (Map and Diagram for all hit reactions) RXL ---- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS ----- Hit Reaction Summariers (Map and Summary for all hit reactions) SPATH ----- Reaction Map/and Reaction Diagram for the "short path". Displays all single step reactions which contain a Mit substance. Also displays those multistep feactions that have a hit substance in both the first/and last steps of the reaction, except for those hit/reactions whose steps are totally included within another hit reaction which is displayed To display a particular field or fields, enter the display field

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):

ENTER DISPLAY FORMAT (FCRDREF): fhit cbib abs

L59 ANSWER 1 OF 1 CASREACT COPYRIGHT 2001 ACS

RX(11) OF 12 COMPOSED OF RX(3), RX(7)RX(11) 2 K + 2 B + Q ===> U

K

K

VIELD 83%

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RX (3)
          RCT K 231957-27-0
            STAGE (1)
               RGT E 683-18-1 Bu2SnCl2, F 7087-68-5 EtN(Pr-i)2
                   107-06-2 ClCH2CH2Cl
          STAGE(2)
               RCT B 54314-83-9
              L 289891-45-8, M 289891-49-2
          NTE regioselective key step
RX (7)
          RCT L 289891-45-8
            STAGE (1)
               RGT F 7087-68-5 EtN(Pr-i)2
               SOL 75-09-2 CH2C12
            STAGE (2)
               RCT 0 89992-70-1
              U 289891-53-8
          NTE (1:1 diastereomeric mixt.)
133:208110 Synthesis of 5'-C- and 2'-O-(bromoalkyl)-substituted
ribonucleoside
     phosphoramidites for the post-synthetic functionalization of
     oligonucleotides on solid support. Wu, Xiaolin; Pitsch, Stefan
     (Laboratorium fur Organische Chemie, ETH-Zentrum, Zurich, CH-8092,
     Switz.). Helv. Chim. Acta, 83(6), 1127-1144 (English) 2000. CODEN:
     HCACAV. ISSN: 0018-019X. Publisher: Verlag Helvetica Chimica Acta.
     The prepn. of building blocks for the incorporation of
AB
     6'-O-(5-bromopenty1)-substituted .beta.-D-allofuranosylnucleosides and
```

2'-O-[(3-bromopropoxy)methyl]-substituted ribonucleosides into

oligonucleotide sequences is presented. These reactive building blocks can be modified with a variety of soft nucleophiles while the (fully Prepared by M. Hale 308-4258 Page 263

protected) sequence is still attached to the solid support. As an example  $\ensuremath{\mathsf{e}}$ 

of this strategy, we carried out some preliminary solid-phase substitution  ${\ }$ 

and conjugation reactions with DNA sequences contg. a 2'-O-[(3-bromopropoxy)methyl]-substituted ribonucleoside and detd. the pairing properties of duplexes obtained therefrom.

## => log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	95.69	3801.61
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.56	-16.44

STN INTERNATIONAL LOGOFF AT 14:12:33 ON 06 APR 2001

=> d 12 que stat; s 12 or 12

L1

STR

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VAR G2=32-4 33-30/34-4 35-30/38-4 40-30/N/O/S/SE/44-4 45-30/HY/50-4 54-30
VAR G3=32-6 33-31/34-6 35-31/38-6 40-31/44-6 45-31/N/O/S/SE/HY/50-6 54-31

NODE ATTRIBUTES:

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GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 33

STEREO ATTRIBUTES: NONE

L2 18919 SEA FILE=REGISTRY SSS FUL L1

9.2% PROCESSED 472964 ITERATIONS

18919 ANSWERS

Page 1

SEARCH TIME: 00.00.44

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9000 RN 147929-45-1 REGISTRY 18000 RN 77926-16-0 REGISTRY

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L4
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          9803 L2 OR L2
L5
=> del 15 y;s 13 range=(77926-16-0,147929-45-1)
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L5
=> s 13 range=(,77926-16-0)
           920 L2 OR L2
L6
=> act garciapt2/a
L7
                 STR
            5070 SEA FILE=REGISTRY SSS FUL L7
L8
=> act garciapt3/a
L9
            314 SEA FILE=REGISTRY SSS FUL L9
L10
=> d 18 que stat;d 110 que stat;fil medl,caplus,biosis,embase;s 110 and 18
L7
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                                46
                                                  48
                                                  0
               N\sim\sim O
  N \sim N
                                                  $@44
                                 539
 @32 @33
              @34 @35
                             NH~S~NH
                                                \sim P\sim 0
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                                             0
                                 0~ C~ CH2 C~ O
                                @53 54 55 56 @57
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NSPEC IS RC

AT 29

NSPEC IS RC A

Prepared by M. Hale 308-4258

Page 2

DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 34

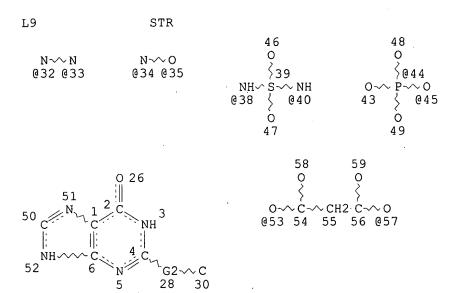
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5070 ANSWERS



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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 33.

STEREO ATTRIBUTES: NONE

L10 314 SEA FILE=REGISTRY SSS FUL L9

100.0% PROCESSED 78598 ITERATIONS

SEARCH TIME: 00.00.16

314 ANSWERS